

10/ 829,064

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NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	FEB 25	CA/CAPLUS - Russian Agency for Patents and Trademarks (ROSPATENT) added to list of core patent offices covered
NEWS	4	FEB 28	PATDPAFULL - New display fields provide for legal status data from INPADOC
NEWS	5	FEB 28	BABS - Current-awareness alerts (SDIs) available
NEWS	6	FEB 28	MEDLINE/LMEDLINE reloaded
NEWS	7	MAR 02	GBFULL: New full-text patent database on STN
NEWS	8	MAR 03	REGISTRY/ZREGISTRY - Sequence annotations enhanced
NEWS	9	MAR 03	MEDLINE file segment of TOXCENTER reloaded
NEWS	10	MAR 22	KOREAPAT now updated monthly; patent information enhanced
NEWS	11	MAR 22	Original IDE display format returns to REGISTRY/ZREGISTRY
NEWS	12	MAR 22	PATDPASPC - New patent database available
NEWS	13	MAR 22	REGISTRY/ZREGISTRY enhanced with experimental property tags
NEWS	14	APR 04	EPFULL enhanced with additional patent information and new fields
NEWS	15	APR 04	EMBASE - Database reloaded and enhanced
NEWS	16	APR 18	New CAS Information Use Policies available online
NEWS	17	APR 25	Patent searching, including current-awareness alerts (SDIs), based on application date in CA/CAPLUS and USPATFULL/USPAT2 may be affected by a change in filing date for U.S. applications.
NEWS	18	APR 28	Improved searching of U.S. Patent Classifications for U.S. patent records in CA/CAPLUS
NEWS EXPRESS			JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005
NEWS HOURS			STN Operating Hours Plus Help Desk Availability
NEWS INTER			General Internet Information
NEWS LOGIN			Welcome Banner and News Items
NEWS PHONE			Direct Dial and Telecommunication Network Access to STN
NEWS WWW			CAS World Wide Web Site (general information)

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10/ 829,064

***** STN Columbus *****

FILE 'HOME' ENTERED AT 17:11:03 ON 05 MAY 2005

=> file reg

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
0.21	0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 17:11:12 ON 05 MAY 2005

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STRUCTURE FILE UPDATES: 4 MAY 2005 HIGHEST RN 849790-35-8

DICTIONARY FILE UPDATES: 4 MAY 2005 HIGHEST RN 849790-35-8

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TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

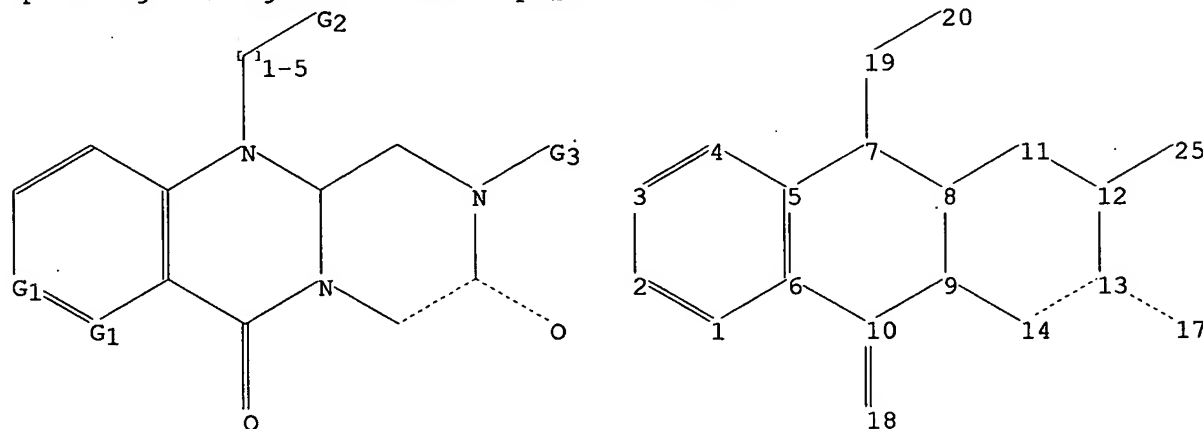
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10829064.str



10/ 829,064

chain nodes :

17 18 19 20 25

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14

chain bonds :

7-19 10-18 12-25 13-17 19-20

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 8-11 9-10 9-14 11-12 12-13 13-14

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-19 9-14 10-18 12-25 13-14 13-17 19-20

exact bonds :

5-7 6-10 7-8 8-9 8-11 9-10 11-12 12-13

isolated ring systems :

containing 1 :

G1:C,N

G2:Ph,Hy

G3:Cb,Ak

Match level :

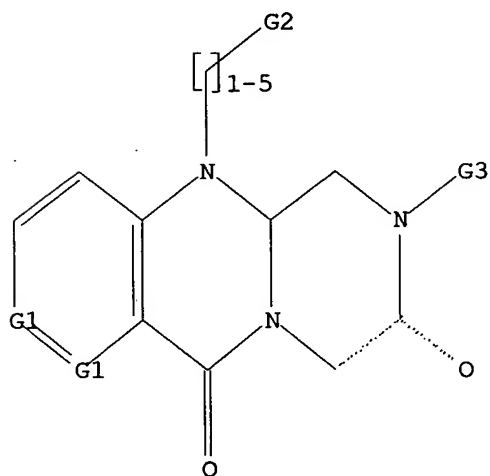
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 17:Atom 18:Atom 19:CLASS 20:CLASS 25:CLASS

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR



G1 C,N

G2 Ph,Hy

G3 Cb,Ak

Structure attributes must be viewed using STN Express query preparation.

10/ 829,064

=> s l1 sample

SAMPLE SEARCH INITIATED 17:11:38 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 5 TO ITERATE

100.0% PROCESSED 5 ITERATIONS 3 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 5 TO 234
PROJECTED ANSWERS: 3 TO 163

L2 3 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 17:11:44 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 158 TO ITERATE

100.0% PROCESSED 158 ITERATIONS 61 ANSWERS
SEARCH TIME: 00.00.01

L3 61 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	161.33	161.54

FILE 'CAPLUS' ENTERED AT 17:11:49 ON 05 MAY 2005
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FILE COVERS 1907 - 5 May 2005 VOL 142 ISS 19
FILE LAST UPDATED: 4 May 2005 (20050504/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3

L4 2 L3

=> d his

(FILE 'HOME' ENTERED AT 17:11:03 ON 05 MAY 2005)

10/ 829,064

FILE 'REGISTRY' ENTERED AT 17:11:12 ON 05 MAY 2005

L1 STRUCTURE UPLOADED

L2 3 S L1 SAMPLE

L3 61 S L1 FULL

FILE 'CAPLUS' ENTERED AT 17:11:49 ON 05 MAY 2005

L4 2 S L3

=> d l4 1- ibib abs hitstr

YOU HAVE REQUESTED DATA FROM 2 ANSWERS - CONTINUE? Y/(N):y

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:898609 CAPLUS

DOCUMENT NUMBER: 141:366248

TITLE: A preparation of triaza- and tetraazaanthracenedione derivatives, useful as cardiovascular agents
 INVENTOR(S): Weichert, Andreas; Strobel, Hartmut; Wohlfart, Paulus;
 Patek, Marcel; Sarcina, Martin; Weichsel, Aleksandra

PATENT ASSIGNEE(S): Aventis Pharma Deutschland GmbH, Germany

SOURCE: Eur. Pat. Appl., 32 pp.

CODEN: EPXKXW

DOCUMENT TYPE: Patent

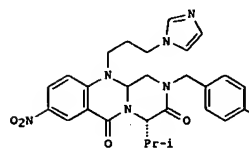
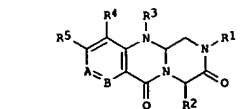
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1471066	A1	20041027	EP 2003-9286	20030424
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
WO 2004094425	A1	20041104	WO 2004-EP3851	20040413
V: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GV, HL, HR, NE, SN, TD, TG				
US 2004248900	A1	20041209	US 2004-829064	20040421
PRIORITY APPL. INFO.:			EP 2003-9286	A 20030424
			US 2003-499521P	P 20030902
OTHER SOURCE(S):		MARPAT 141:366248		
GI				

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



AB The invention relates to a preparation of triaza- and tetraaza-anthracenedione derivs. of formula I (wherein: A and B are independently selected from N, CH, C-halogen, C-NO₂, or C-CN, etc., but A and B are not simultaneously N; R1 is (un)substituted (cyclo)alkyl or alk(en/yn)yl; R2 is H, alkyl, CF₃, or (CH₂)₀₋₂ (phenyl/imidazolyl), etc.; R3 is (CH₂)₁₋₄ (phenyl/imidazolyl/triazolyl) or (CH₂)₁₋₄ pyridinyl, etc.; R4 and R5 are independently selected from H, alkyl, CF₃, or alkoxy, etc.), useful as cardiovascular agents. The title compds. are useful in the treatment of various disease states including cardiovascular disorders such as atherosclerosis, thrombosis, coronary artery disease, hypertension, and cardiac insufficiency. They upregulate the expression of the enzyme endothelial nitric oxide (NO) synthase and can be applied in conditions in which an increased expression of said enzyme or an increased NO level or the normalization of a decreased NO level is desired. For instance, triazaanthracenedione derivative II (activation of eNOS transcription: EC50

1.2 μM) was prepared via heterocyclization of 4-tert-butylbenzylamine, Fmoc-L-valine, 2-fluoro-5-nitrobenzoic acid, 2-bromo-1,1-diethoxyethane, and 3-(imidazol-1-yl)propylamine (example 2, no yield data).

IT 779343-75-OP 779343-77-OP 779343-79-2P
 779343-81-OP 779343-83-OP 779343-85-OP
 779343-87-2P 779343-89-4P 779343-93-OP
 779343-95-2P 779343-97-4P 779343-99-6P
 779344-01-3P 779344-03-5P 779344-05-7P
 779344-07-9P 779344-08-OP 779344-09-1P
 779344-10-4P 779344-11-5P 779344-12-6P
 779344-13-7P 779344-14-8P 779344-15-9P
 779344-16-OP 779344-17-1P 779344-18-2P
 779344-19-3P 779344-20-6P 779344-21-7P
 779344-22-8P 779344-23-9P 779344-24-OP
 779344-25-1P 779344-27-3P 779344-29-5P
 779344-32-OP 779344-34-2P 779344-36-4P

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOD (Biological study); PREP (Preparation); USES (Uses)

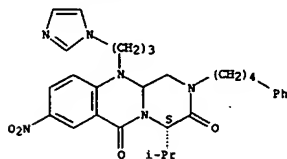
(prepn. of triaza- and tetraaza-anthracenedione derivs., useful as cardiovascular agents)

RN 779343-75-8 CAPLUS
 CN GH-Pyrazino[2,1-b]quinazoline-3,6(4H)-dione, 1,2,11,11a-tetrahydro-11-[(3-(1H-imidazol-1-yl)propyl)-4-(1-methylethyl)-8-nitro-2-(4-phenylbutyl)-, (4S)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 779343-74-7
 CMF C30 H36 N6 O4

Absolute stereochemistry.



CM 2

CRN 76-05-1
 CMF C2 H F3 O2



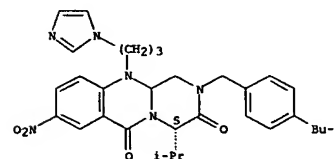
RN 779343-77-0 CAPLUS
 CN GH-Pyrazino[2,1-b]quinazoline-3,6(4H)-dione, 2-[[[4-(1,1-dimethylethyl)phenyl]methyl]-1,2,11,11a-tetrahydro-11-[(3-(1H-imidazol-1-yl)propyl)-4-(1-methylethyl)-8-nitro-, (4S)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 779343-76-9
 CMF C31 H38 N6 O4

Absolute stereochemistry.

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



CM 2

CRN 76-05-1
 CMF C2 H F3 O2

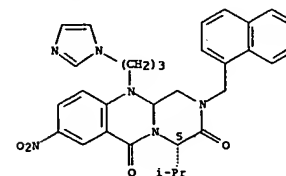


RN 779343-79-2 CAPLUS
 CN GH-Pyrazino[2,1-b]quinazoline-3,6(4H)-dione, 1,2,11,11a-tetrahydro-11-[(3-(1H-imidazol-1-yl)propyl)-4-(1-methylethyl)-2-(1-naphthalenylmethyl)-8-nitro-, (4S)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 779343-78-1
 CMF C31 H32 N6 O4

Absolute stereochemistry.



CM 2

CRN 76-05-1
 CMF C2 H F3 O2

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

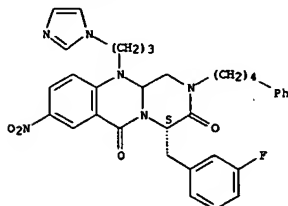


RN 779343-81-6 CAPLUS
 CN 6H-Pyrazino[2,1-b]quinazoline-3,6(4H)-dione, 4-[(3-fluorophenyl)methyl]-1,2,11,11a-tetrahydro-11-[3-(1H-imidazol-1-yl)propyl]-8-nitro-2-(4-phenylbutyl)-, (4S)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CH 1

CRN 779343-80-5
 CMF C34 H35 F N6 O4

Absolute stereochemistry.



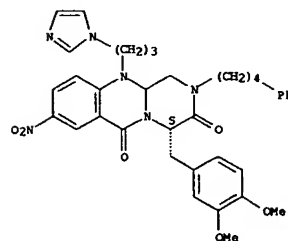
CH 2

CRN 76-05-1
 CMF C2 H F3 O2



RN 779343-83-8 CAPLUS
 CN 6H-Pyrazino[2,1-b]quinazoline-3,6(4H)-dione, 4-cyclohexyl-1,2,11,11a-tetrahydro-11-[3-(1H-imidazol-1-yl)propyl]-8-nitro-2-(4-phenylbutyl)-, (4S)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



CH 2

CRN 76-05-1
 CMF C2 H F3 O2



RN 779343-87-2 CAPLUS
 CN 6H-Pyrazino[2,1-b]quinazoline-3,6(4H)-dione, 1,2,11,11a-tetrahydro-4-(1-methylethyl)-8-nitro-2-(4-phenylbutyl)-11-[2-(4-pyridinyl)ethyl]-, (4S)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CH 1

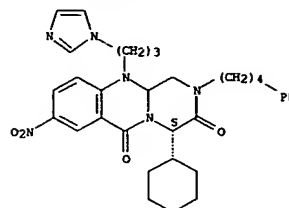
CRN 779343-86-1
 CMF C31 H35 N5 O4

Absolute stereochemistry.

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

CRN 779343-82-7
 CMF C33 H40 N6 O4

Absolute stereochemistry.



CH 2

CRN 76-05-1
 CMF C2 H F3 O2



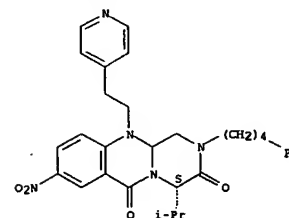
RN 779343-85-0 CAPLUS
 CN 6H-Pyrazino[2,1-b]quinazoline-3,6(4H)-dione, 4-[(3,4-dimethoxyphenyl)methyl]-1,2,11,11a-tetrahydro-11-[3-(1H-imidazol-1-yl)propyl]-8-nitro-2-(4-phenylbutyl)-, (4S)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CH 1

CRN 779343-84-9
 CMF C36 H40 N6 O6

Absolute stereochemistry.

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



CH 2

CRN 76-05-1
 CMF C2 H F3 O2

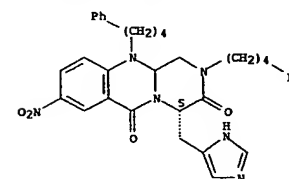


RN 779343-89-4 CAPLUS
 CN 6H-Pyrazino[2,1-b]quinazoline-3,6(4H)-dione, 1,2,11,11a-tetrahydro-4-(1H-imidazol-4-ylmethyl)-8-nitro-2,11-bis(4-phenylbutyl)-, (4S)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CH 1

CRN 779343-88-3
 CMF C35 H38 N6 O4

Absolute stereochemistry.



L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
 CH 2

CRN 76-05-1
 CHF C2 H F3 O2

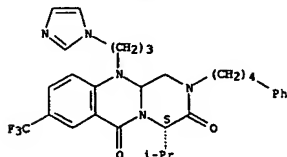


RN 779343-93-0 CAPLUS
 CN 6H-Pyrazino[2,1-b]quinazoline-3,6(4H)-dione, 1,2,11,11a-tetrahydro-11-[3-(1H-imidazol-1-yl)propyl]-4-(1-methylethyl)-2-(4-phenylbutyl)-8-(trifluoromethyl)-, (4S)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CH 1

CRN 779343-92-9
 CHF C31 H36 F3 N5 O2

Absolute stereochemistry.



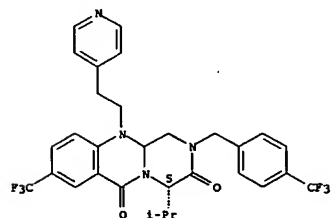
CH 2

CRN 76-05-1
 CHF C2 H F3 O2



RN 779343-95-2 CAPLUS
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L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



CH 2

CRN 76-05-1
 CHF C2 H F3 O2

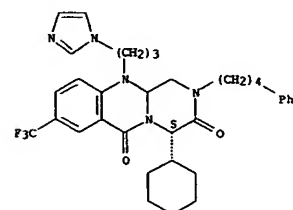


RN 779343-99-6 CAPLUS
 CN 6H-Pyrazino[2,1-b]quinazoline-3,6(4H)-dione, 4-cyclohexyl-1,2,11,11a-tetrahydro-11-[3-(1H-imidazol-1-yl)propyl]-2-(4-phenylbutyl)-8-(trifluoromethyl)-, (4S)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CH 1

CRN 779343-98-5
 CHF C34 H40 F3 N5 O2

Absolute stereochemistry.

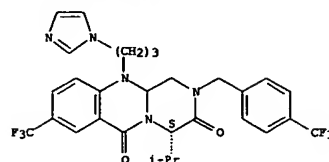


L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
 INDEX NAME

CH 1

CRN 779343-94-1
 CHF C29 H29 F6 N5 O2

Absolute stereochemistry.



CH 2

CRN 76-05-1
 CHF C2 H F3 O2



RN 779343-97-4 CAPLUS
 CN 6H-Pyrazino[2,1-b]quinazoline-3,6(4H)-dione, 1,2,11,11a-tetrahydro-4-(1-methylethyl)-11-[2-(4-pyridinyl)ethyl]-8-(trifluoromethyl)-2-[[4-(trifluoromethyl)phenyl]methyl]-, (4S)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CH 1

CRN 779343-96-3
 CHF C30 H28 F6 N4 O2

Absolute stereochemistry.

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

CH 2

CRN 76-05-1
 CHF C2 H F3 O2

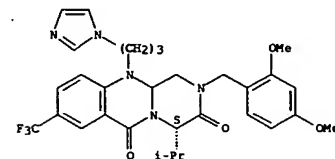


RN 779344-01-3 CAPLUS
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CH 1

CRN 779344-00-2
 CHF C30 H34 F3 N5 O4

Absolute stereochemistry.



CH 2

CRN 76-05-1
 CHF C2 H F3 O2



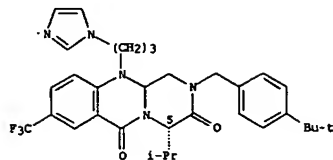
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L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

CM 1

CRN 779344-02-4
CMF C32 H38 F3 N5 O2

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2

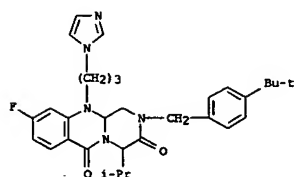
RN 779344-05-7 CAPLUS
CN 6H-Pyrazino[2,1-b]quinazoline-3,6(4H)-dione, 4-[(3-fluorophenyl)methyl]-1,2,11,11a-tetrahydro-11-[3-(1H-imidazol-1-yl)propyl]-2-(4-phenylbutyl)-8-(trifluoromethyl)-, (4S)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 779344-04-6
CMF C35 H35 F4 N5 O2

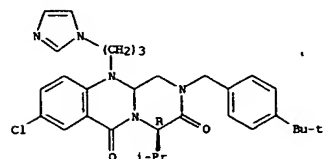
Absolute stereochemistry.

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



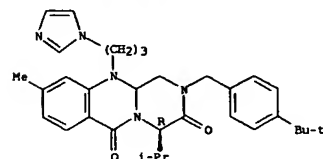
RN 779344-09-1 CAPLUS
CN 2H-Pyrazino[2,1-b]quinazoline-3,6(1H,4H)-dione, 8-chloro-2-[[4-(1,1-dimethylethyl)phenyl]methyl]-11,11a-dihydro-11-[3-(1H-imidazol-1-yl)propyl]-4-(1-methylethyl)-, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



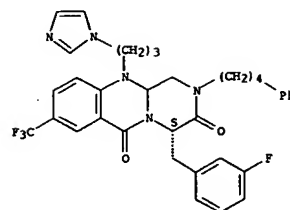
RN 779344-10-4 CAPLUS
CN 2H-Pyrazino[2,1-b]quinazoline-3,6(1H,4H)-dione, 2-[[4-(1,1-dimethylethyl)phenyl]methyl]-11,11a-dihydro-11-[3-(1H-imidazol-1-yl)propyl]-9-methyl-4-(1-methylethyl)-, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 779344-11-5 CAPLUS
CN 2H-Pyrazino[2,1-b]quinazoline-3,6(1H,4H)-dione, 2-[[4-(1,1-dimethylethyl)phenyl]methyl]-11,11a-dihydro-11-[3-(1H-imidazol-1-yl)propyl]-8-methoxy-4-(1-methylethyl)-, (4R)- (9CI) (CA INDEX NAME)

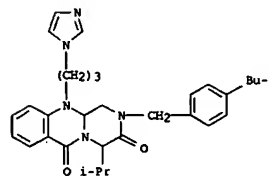
L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



CM 2

CRN 76-05-1
CMF C2 H F3 O2

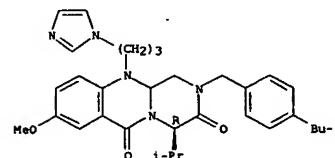
RN 779344-07-9 CAPLUS
CN 2H-Pyrazino[2,1-b]quinazoline-3,6(1H,4H)-dione, 2-[[4-(1,1-dimethylethyl)phenyl]methyl]-11,11a-dihydro-11-[3-(1H-imidazol-1-yl)propyl]-4-(1-methylethyl)- (9CI) (CA INDEX NAME)



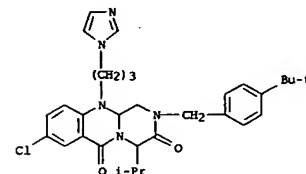
RN 779344-08-0 CAPLUS
CN 2H-Pyrazino[2,1-b]quinazoline-3,6(1H,4H)-dione, 2-[[4-(1,1-dimethylethyl)phenyl]methyl]-9-fluoro-11,11a-dihydro-11-[3-(1H-imidazol-1-yl)propyl]-4-(1-methylethyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

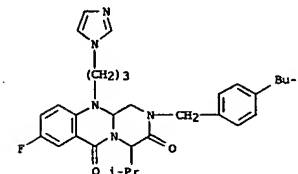
Absolute stereochemistry.



RN 779344-12-6 CAPLUS
CN 2H-Pyrazino[2,1-b]quinazoline-3,6(1H,4H)-dione, 8-chloro-2-[[4-(1,1-dimethylethyl)phenyl]methyl]-11,11a-dihydro-11-[3-(1H-imidazol-1-yl)propyl]-4-(1-methylethyl)- (9CI) (CA INDEX NAME)

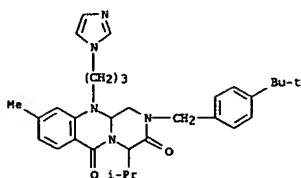


RN 779344-13-7 CAPLUS
CN 2H-Pyrazino[2,1-b]quinazoline-3,6(1H,4H)-dione, 2-[[4-(1,1-dimethylethyl)phenyl]methyl]-8-fluoro-11,11a-dihydro-11-[3-(1H-imidazol-1-yl)propyl]-4-(1-methylethyl)- (9CI) (CA INDEX NAME)

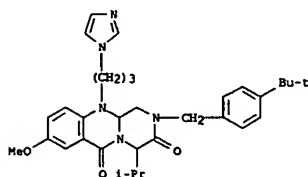


RN 779344-14-8 CAPLUS
CN 2H-Pyrazino[2,1-b]quinazoline-3,6(1H,4H)-dione, 2-[[4-(1,1-dimethylethyl)phenyl]methyl]-11,11a-dihydro-11-[3-(1H-imidazol-1-yl)propyl]-9-methyl-4-(1-methylethyl)- (9CI) (CA INDEX NAME)

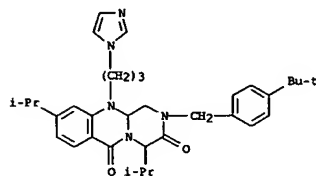
L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



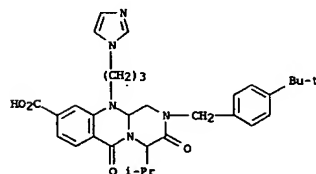
RN 779344-15-9 CAPLUS
CN 2H-Pyrazino[2,1-b]quinazoline-3,6(1H,4H)-dione, 2-[[4-(1,1-dimethylethyl)phenyl]methyl]-11,11a-dihydro-11-[3-(1H-imidazol-1-yl)propyl]-8-methoxy-4-(1-methylethyl)- (9CI) (CA INDEX NAME)



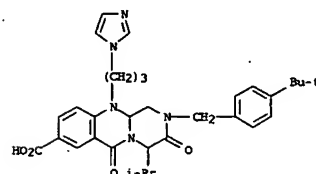
RN 779344-16-0 CAPLUS
CN 2H-Pyrazino[2,1-b]quinazoline-3,6(1H,4H)-dione, 2-[[4-(1,1-dimethylethyl)phenyl]methyl]-11,11a-dihydro-11-[3-(1H-imidazol-1-yl)propyl]-4,9-bis(1-methylethyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

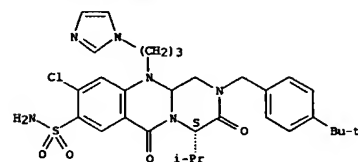


RN 779344-20-6 CAPLUS
CN 2H-Pyrazino[2,1-b]quinazoline-8-carboxylic acid, 2-[[4-(1,1-dimethylethyl)phenyl]methyl]-1,3,4,6,11,11a-hexahydro-11-[3-(1H-imidazol-1-yl)propyl]-4-(1-methylethyl)-3,6-dioxo- (9CI) (CA INDEX NAME)



RN 779344-21-7 CAPLUS
CN 2H-Pyrazino[2,1-b]quinazoline-8-sulfonamide, 9-chloro-2-[[4-(1,1-dimethylethyl)phenyl]methyl]-1,3,4,6,11,11a-hexahydro-11-[3-(1H-imidazol-1-yl)propyl]-4-(1-methylethyl)-3,6-dioxo-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

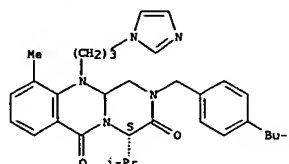


RN 779344-22-8 CAPLUS
CN 2H-Pyrazino[2,1-b]quinazoline-8-sulfonamide, 2-[[4-(1,1-dimethylethyl)phenyl]methyl]-1,3,4,6,11,11a-hexahydro-11-[3-(1H-imidazol-1-yl)propyl]-N-methyl-4-(1-methylethyl)-3,6-dioxo-, (4S)- (9CI) (CA INDEX NAME)

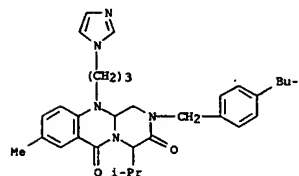
L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 779344-17-1 CAPLUS
CN 2H-Pyrazino[2,1-b]quinazoline-3,6(1H,4H)-dione, 2-[[4-(1,1-dimethylethyl)phenyl]methyl]-11,11a-dihydro-11-[3-(1H-imidazol-1-yl)propyl]-10-methyl-4-(1-methylethyl)-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



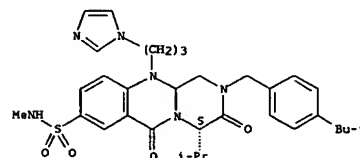
RN 779344-18-2 CAPLUS
CN 2H-Pyrazino[2,1-b]quinazoline-3,6(1H,4H)-dione, 2-[[4-(1,1-dimethylethyl)phenyl]methyl]-11,11a-dihydro-11-[3-(1H-imidazol-1-yl)propyl]-8-methyl-4-(1-methylethyl)- (9CI) (CA INDEX NAME)



RN 779344-19-3 CAPLUS
CN 2H-Pyrazino[2,1-b]quinazoline-9-carboxylic acid, 2-[[4-(1,1-dimethylethyl)phenyl]methyl]-1,3,4,6,11,11a-hexahydro-11-[3-(1H-imidazol-1-yl)propyl]-4-(1-methylethyl)-3,6-dioxo- (9CI) (CA INDEX NAME)

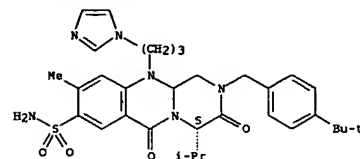
L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

Absolute stereochemistry.



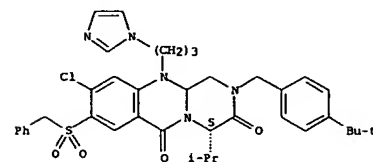
RN 779344-23-9 CAPLUS
CN 2H-Pyrazino[2,1-b]quinazoline-8-sulfonamide, 2-[[4-(1,1-dimethylethyl)phenyl]methyl]-1,3,4,6,11,11a-hexahydro-11-[3-(1H-imidazol-1-yl)propyl]-9-methyl-4-(1-methylethyl)-3,6-dioxo-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 779344-24-0 CAPLUS
CN 2H-Pyrazino[2,1-b]quinazoline-3,6(1H,4H)-dione, 9-chloro-2-[[4-(1,1-dimethylethyl)phenyl]methyl]-11,11a-dihydro-11-[3-(1H-imidazol-1-yl)propyl]-4-(1-methylethyl)-8-[(phenylmethyl)sulfonyl]-, (4S)- (9CI) (CA INDEX NAME)

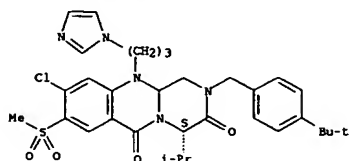
Absolute stereochemistry.



RN 779344-25-1 CAPLUS
CN 2H-Pyrazino[2,1-b]quinazoline-3,6(1H,4H)-dione, 9-chloro-2-[[4-(1,1-

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
dimethylethyl)phenyl)methyl]-11,11a-dihydro-11-[3-(1H-imidazol-1-yl)propyl]-4-(1-methylethyl)-8-(methylsulfonyl)-, (4S)- (9CI) (CA INDEX NAME)

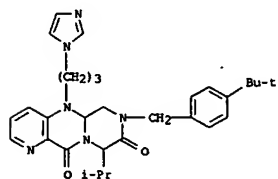
Absolute stereochemistry.



RN 779344-27-3 CAPLUS
CN 7H-Pyrazino[1,2-a]pyrido[3,2-d]pyrimidine-8,11(5H,9H)-dione, 7-[[4-[(1,1-dimethylethyl)phenyl)methyl]-5a,6-dihydro-5-[3-(1H-imidazol-1-yl)propyl]-9-(1-methylethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CH 1

CRN 779344-26-2
CHF C30 H39 N6 O2

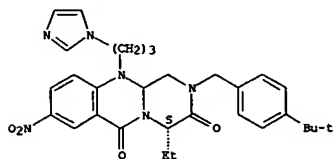


CH 2

CRN 76-05-1
CHF C2 H F3 O2

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
CRN 779344-31-9
CHF C30 H36 N6 O4

Absolute stereochemistry.



CH 2

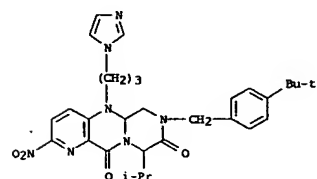
CRN 76-05-1
CHF C2 H F3 O2



RN 779344-34-2 CAPLUS
CN 7H-Pyrazino[1,2-a]pyrido[3,2-d]pyrimidine-8,11(5H,9H)-dione, 7-[[4-[(1,1-dimethylethyl)phenyl)methyl]-5a,6-dihydro-5-[3-(1H-imidazol-1-yl)propyl]-9-(1-methylethyl)-2-nitro-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CH 1

CRN 779344-33-1
CHF C30 H37 N7 O4



CH 2

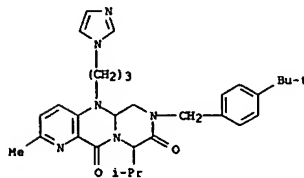
L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



RN 779344-29-5 CAPLUS
CN 7H-Pyrazino[1,2-a]pyrido[3,2-d]pyrimidine-8,11(5H,9H)-dione, 7-[[4-[(1,1-dimethylethyl)phenyl)methyl]-5a,6-dihydro-5-[3-(1H-imidazol-1-yl)propyl]-9-(1-methylethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CH 1

CRN 779344-28-4
CHF C31 H40 N6 O2



CH 2

CRN 76-05-1
CHF C2 H F3 O2



RN 779344-32-0 CAPLUS
CN 6H-Pyrazino[2,1-b]quinazoline-3,6(4H)-dione, 2-[[4-[(1,1-dimethylethyl)phenyl)methyl]-4-ethyl-1,2,11,11a-tetrahydro-11-[3-(1H-imidazol-1-yl)propyl]-8-nitro-, (4S)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CH 1

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

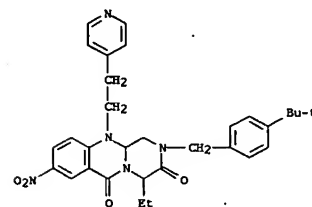
CRN 76-05-1
CHF C2 H F3 O2



RN 779344-36-4 CAPLUS
CN 6H-Pyrazino[2,1-b]quinazoline-3,6(4H)-dione, 2-[[4-[(1,1-dimethylethyl)phenyl)methyl]-4-ethyl-1,2,11,11a-tetrahydro-8-nitro-11-[2-(4-pyridinyl)ethyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CH 1

CRN 779344-35-3
CHF C31 H35 N5 O4



CH 2

CRN 76-05-1
CHF C2 H F3 O2



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:529844 CAPLUS

DOCUMENT NUMBER: 131:286484

TITLE: Synthesis and stereochemistry of 11,11a-dihydro

derivatives of (4S)-2,4-dimethyl-2,4-dihydro-1H-

pyrazino[2,1-b]quinazoline-3,6-diones. A new

transannular rearrangement proposal

Martin-Santamaria, Sonsoles; Espada, Modesta;

Avendano, Carmen

AUTHOR(S):

CORPORATE SOURCE:

Departamento de Quimica Organica y Farmaceutica

Facultad de Farmacia, Universidad Complutense, Madrid,

28040, Spain

SOURCE:

Journal of Organic Chemistry (1999), 64(19), 7233-7235

CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER:

American Chemical Society

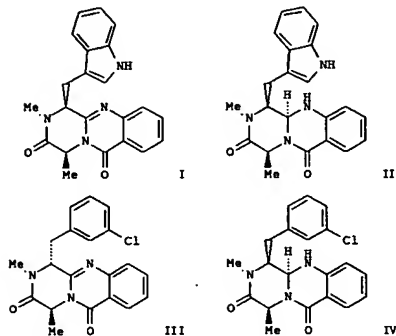
DOCUMENT TYPE:

Journal

LANGUAGE:

English

GI



AB Reduction of the (indolylmethyl)dihydropyrazinoquinazolinone I by NaBH₄/EtOH gave the tetrahydropyrazinoquinazolinone II, whereas similar reduction of (chlorobenzyl)dihydropyrazinoquinazolinone III gave the tetrahydropyrazinoquinazolinone with epimerization at C-1. A proposed mechanism for the epimerization involved transannular rearrangement and formation of a ten-membered-ring anion intermediate.

17 246542-03-OP 246542-05-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

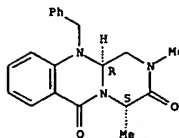
(transannular rearrangement mechanism in borohydride reduction/epimerization of dihydromethylpyrazinoquinazolinones)

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

RN 246542-03-0 CAPLUS

CN ZH-Pyrazino[2,1-b]quinazoline-3,6(1H,4H)-dione, 11,11a-dihydro-2,4-dimethyl-11-(phenylmethyl)-, (4S,11aR)- (9CI) (CA INDEX NAME)

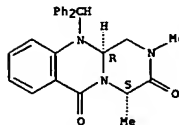
Absolute stereochemistry. Rotation (-).



RN 246542-05-2 CAPLUS

CN ZH-Pyrazino[2,1-b]quinazoline-3,6(1H,4H)-dione, 11-(diphenylmethyl)-11,11a-dihydro-2,4-dimethyl-, (4S,11aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT:

16

THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT